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Numerical approximation of a compressible multiphase system

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Abstract. The numerical simulation of non conservative system is a difficult challenge for two reasons at least. The first one is that it is not possible to derive jump relations directly from conservation principles, so that in general, if the model description is non ambiguous for smooth solutions, this is no longer the case for discontinuous solutions. From the numerical view point, this leads to the following situation: if a scheme is stable, its limit for mesh convergence will depend on its dissipative structure. This is well known since at least [**?**]. In this paper we are interested in the "dual" problem: given a system in non conservative form *and* consistent jump relations, how can we construct a numerical scheme that will, for mesh convergence, provide limit solutions that are the exact solution of the problem. In order to investigate this problem, we consider a multiphase flow model for which jump relations are known. Our scheme is an hybridation of Glimm scheme and Roe scheme.

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Key words: Non conservative systems, numerical approximation, Glimm' scheme, Roe'scheme

Nomenclature.

- α_i : volume fraction of phase i;
- ρ_i: density of phase i; $\rho = \sum_i \alpha_i \rho_i$: average density,
- $\tau_i = 1/\rho_i$: specific volume of phase i; $\tau = 1/\rho$: specific volume,
- $Y_i = \frac{\alpha_i \rho_i}{\rho}$: mass fraction of phase i;
- u: average velocity;
- p: pressure, p_i pressure of phase i;
- s specific entropy, s_i specific entropy of phase i, $s = \sum_i Y_i s_i$;
- ε_i: specific internal energy of phase i;
- e_i: internal energy of phase i, $e_i = \rho_i \varepsilon_i$;
- T_i: temperature of phase i;

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- $e = \sum_i \alpha_i e_i$: internal energy; $E = e + \frac{1}{2}\rho u^2$: total energy
- $\kappa_i = \dfrac{\partial p_i}{\partial e_i}$, $\chi_i = \dfrac{\partial p_i}{\partial \rho_i}$;
- a: speed of sound, a_i speed of sound of phase i.

1 Introduction

In many applications, one needs to consider compressible flows where the fluid is made of several non mixable phases. Examples can been found in the nuclear industry, the oil industry, for engines, etc. Another class of applications can be found in the case of high explosives. In that case, the media is made of several non mixable materials that are so intimately mixed that their exchange surface is very large. Such a fluid can be modeled by two compressible fluids, each having its own equation of state, thus its own pressure and possibly its own velocity. However, in the case of a large inter-facial area, it is legitimate to assume that the phase pressures and velocities are identical. The same situation occur for atomized flows.

The model in this case cannot be the simple model of two mass conservation equations (one for each phase), the momentum conservation equation, a total energy equation and a last one describing the evolution of the fluid composition written as a simple transport equation. In fact, in the physical model, one may encounter smooth variations of the volume fractions. In that case, when a shock wave is moving, this implies that the fluids can be compressed according to their acoustic impedance. A model that describes such a situation is the Kapila model [**?**] which can be derived from variants of the Baer and Nunziato [**?**] model by means of asymptotic expansions, see [**?**]. Here the small parameter is related to the inverse of the inter-facial area. The system of PDEs of the Kapila model is given in section 2. It is written in non conservation form, hence it cannot describe the structure of shock waves: the classical Rankine-Hugoniot relations do not hold, and the derivation of jump relation cannot be obtained using the standard techniques.

However, in [**?**], R. Saurel and coauthors have derived from some heuristic arguments a series of jump relations. Basically, for n phase flows, one has for each phase the classical Hugoniot relations, supplemented by the fact one has a single pressure. These relations satisfies all the requirements, in particular for weak shocks, the Hugoniot curves are tangent to the isentropes. Last, these relations have been validated against numerous experimental test cases with very severe conditions.

From the numerical point of view, for any given Cauchy problem, it is very difficult to construct a method that, under mesh refinement, will provide numerical solutions that are going to converge, in the L^1 norm, to the exact solution. This difficulty occurs because the system (2.1) is written in non conservative form, so that the numerical dissipation of the scheme dictates the limit solution, contrarily to what occurs for systems in conservation form, thanks to Lax-Wendroff theorem. In general, two different discretisations will converge to different solutions, see [**?**] for one explicit example. This problem is not specific to system (2.1), but is typical of non conservative problems.

The question is the following. Given a set of PDEs, and compatible jump relations (see [**?**]), how can we construct a numerical method that will provide sequence of numerical solutions that are guarantied to converge to the exact solution of the problem ? This simple question appears to be quite difficult to solve. The difficulty is to encode in some way the Hugoniot relations in the scheme. Coming back to the system system (2.1), which is one example of such a problem, we are aware of very few solutions, see e.g. [**?**, **?**]. The purpose of the paper is to provide another solution to that problem. Our solution is a combination of the Glimm' scheme and a classical solver. Here we have chosen the Roe scheme, but we believe that our technique can apply to other solvers, and other problems. Using Glim's method and its hybridization with another method to remove noise is not by itself original. For example, Glim' scheme has been advocated for non conservative systems by [?]. To make it work, one needs a Riemann solver, and up to our knowledge, it has never been demonstrated on (2.1) that Glim and its hybridization can actually work. We also test that this strategy is efficient on more complex problem, a nozzle flow with shocks: before and after the internal shock the solution is not constant, and hence one might fear some bad effects in the Riemann solution because the solution is not localy constant.

The paper is organized as follows. We first recall the Kapila model, and its structure. We also provide its Lagrangian form. This form enable to construct a Roe average matrix that can reproduce exactly the Hugoniot relations around a shock, as the classical Roe schemes does for standard compressible flows. We then describe our hybrid scheme, and then numerical examples show the effectiveness of the method. In particular, we are able to produce second order solutions that are oscillation free and noise free (as the pure Glimm' scheme would have produced), even on very strong shock waves. The last case we consider is a nozzle flow problem with a shock in the divergent. In this way we can check whether our procedure is robust since the solution is not constant left and right of the discontinuity.

2 Five equations model

The five equation model, given in Kapila et al. [?] and shown in [?] to be the formal limit of the Baer and Nunziato model when the relaxation parameters simultaneously tends to infinity though being proportional writes:

$$\frac{\partial \alpha_1}{\partial t}+u\cdot\nabla\alpha_1=K\text{div } u, \qquad K:=\frac{\rho_2 a_2^2-\rho_1 a_1^2}{\frac{\rho_1 a_1^2}{\alpha_1}+\frac{\rho_2 a_2^2}{\alpha_2}} \tag{2.1a}$$

$$\frac{\partial(\alpha_1\rho_1)}{\partial t}+\text{ div }(\alpha_1\rho_1 u)=0 \tag{2.1b}$$

$$\frac{\partial(\alpha_2\rho_2)}{\partial t}+\text{ div }(\alpha_2\rho_2 u)=0 \tag{2.1c}$$

$$\frac{\partial(\rho_u)}{\partial t}+\text{ div }(\rho u^2+p)=0 \tag{2.1d}$$

$$\frac{\partial E}{\partial t}+\text{ div }\Big((E+p)u\Big)=0. \tag{2.1e}$$

As usual, the total energy E is the sum of the internal energy $\rho\varepsilon$ and the kinetic energy, ε is the specific internal energy, α_i is the volume fraction of phase i, ρ_i is the density of phase i and u the velocity. The mass is $\rho=\alpha_1\rho_1+\alpha_2\rho_2$. Later in the text, we need the mass fraction of phase i defined by

$$\alpha_i\rho_i=Y_i\rho.$$

As a consequence, we also have $Y_1+Y_2=1$. We also need $\tau_i=1/\rho_i$. In this model, we assume a single pressure. If $p_i=p_i(\rho_i,e_i)$ is the equation of state of phase i, this means that we assume the constraint $p_1(\rho_1,e_1)=p_2(\rho_1,e_2)=p$. This relation, associated to the saturation relation $\alpha_1+\alpha_2=1$, closes the system.

The system (2.1) is an hyperbolic system and hence admits discontinuous solutions. It admits three linearly degenerate fields, associated to the eigenvalue u, and two genuinely non linear fields, associated to the eigenvalues $u \pm a$. The expression of the speed of sound a, also known as the Wallis speed of sound, is given by:

$$\frac{1}{\rho a^2} = \frac{\alpha_1}{\rho_1 a_1^2} + \frac{\alpha_2}{\rho_2 a_2^2}, \tag{2.2}$$

where the speeds a_i are given classically by

$$a_i^2 = \left.\frac{\partial p_i}{\partial \rho_i}\right|_{s_i}.$$

Since the system is hyperbolic, we need to consider discontinuous solutions. In [**?**], Saurel proposes jump relations that writes, where we set as usual $\Delta f = f_L - f_R$ and $\overline{f} = \frac{f_L + f_R}{2}$

$$\Delta Y_1 = 0; \Delta Y_2 = 0 \tag{2.3a}$$

$$\Delta \varepsilon_1 + \overline{p} \Delta \tau_1 = 0 \tag{2.3b}$$

$$\Delta \varepsilon_2 + \overline{p} \Delta \tau_2 = 0 \tag{2.3c}$$

supplemented by

$$\Delta u^2 + \Delta p \Delta \tau = 0. \tag{2.3d}$$

The relations (2.3) , in particular (2.3b) and (2.3c), are the Hugoniot of the pure phase fluids.

3 The Lagrangian form of the equations

3.1 The 5 equations model in Lagrangian coordinates

We start from its form in Eulerian coordinates (2.1). In what follows $\frac{D}{Dt}$ is the Lagrangian derivative.The combination of (2.1b) and (2.1c), combined with the mass coordinate defined by $dm = \rho dx$ leads to (with $\tau = 1/\rho$)

$$\frac{D\tau}{Dt} - \frac{\partial u}{\partial m} = 0.$$

This relation combined with (2.1b) leads to

$$\frac{DY_1}{Dt} = 0$$

The equation on the momentum becomes

$$\frac{Du}{Dt} + \frac{\partial p}{\partial m} = 0$$

The energy equation, defining $e = \varepsilon + \frac{u^2}{2}$ leads to

$$\frac{De}{Dt} + \frac{\partial (pu)}{\partial m} = 0.$$

Last, the equation on the volume fraction becomes

$$\frac{D\alpha_2}{Dt} - \frac{K}{\tau}\frac{\partial u}{\partial m} = 0$$

with

$$K = \frac{\frac{\alpha_2}{Y_2}C_2^2 - \frac{\alpha_1}{Y_1}C_1^2}{\frac{C_1^2}{Y_1} + \frac{C_2^2}{Y_2}} = \frac{\rho_2 a_2^2 - \rho_1 a_1^2}{\frac{\rho_1 a_1^2}{\alpha_1} + \frac{\rho_2 a_2^2}{\alpha_2}}$$

where C_i is the Lagrangian speed of sound and a_i is the Eulerian one.

This relation can be obtained from (2.1a) or, as in [**?**], by taking the Lagrangian derivative of the equality

$$p = p_1(\varepsilon_1, \tau_1) = p_2(\varepsilon_2, \tau_2).$$

To come back to classical notations, we replace the time derivatives by $\frac{\partial}{\partial t}$ and the derivative in the mass coordinate system by $\frac{\partial}{\partial x}$, so that the systems becomes (3.1).

$$\frac{\partial \alpha_1}{\partial t} - \frac{K}{\tau}\frac{\partial u}{\partial x} = 0 \tag{3.1a}$$

$$\frac{dY_1}{dt} = 0 \tag{3.1b}$$

$$\frac{\partial \tau}{\partial t} - \frac{\partial u}{\partial x} = 0 \tag{3.1c}$$

$$\frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} = 0 \tag{3.1d}$$

$$\frac{\partial e}{\partial t} + \frac{\partial (pu)}{\partial x} = 0. \tag{3.1e}$$

Note that the pressure p depends on ε, τ, Y_1 and α_1.

3.2 Structure of the Jacobian matrix

The Jacobian matrix of (3.1) is

$$A = \begin{pmatrix} 0 & 0 & 0 & -K/\tau & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ p_{\alpha_1} & p_{Y_1} & p_\tau & -p_\varepsilon u & p_\varepsilon \\ u p_{\alpha_1} & u p_{Y_1} & u p_\tau & p - p_\varepsilon u^2 & u p_\varepsilon \end{pmatrix}.$$

The characteristic polynomial of A is

$$P(\lambda) = -\lambda^3 \left(\lambda^2 - \left(p_\varepsilon p - p_\tau - \frac{K}{\tau} p_{\alpha_1} \right) \right).$$

There are 3 eigenvalues : $\lambda = 0$ is triple and $\lambda_\pm = \pm C$ with

$$C^2 = p_\varepsilon p - p_\tau - \frac{K}{\tau} p_{\alpha_1}. \tag{3.2}$$

The eigenvectors are

- For the eigenvalue $\lambda = C$,

$$R_1 = \begin{pmatrix} -K/\tau \\ 0 \\ -1 \\ C \\ p+uC \end{pmatrix}$$

- For the eigenvalue $\lambda = -C$,

$$R_1 = \begin{pmatrix} -K/\tau \\ 0 \\ -1 \\ -C \\ p-uC \end{pmatrix}$$

- For the eigenvalue $\lambda = 0$,

$$R_3 = \begin{pmatrix} -p_\varepsilon \\ 0 \\ 0 \\ 0 \\ p_{\alpha_1} \end{pmatrix}, \qquad R_4 = \begin{pmatrix} 0 \\ -p_\varepsilon \\ 0 \\ 0 \\ p_{Y_1} \end{pmatrix}, \qquad R_5 = \begin{pmatrix} 0 \\ 0 \\ -p_\varepsilon \\ 0 \\ p_\tau \end{pmatrix}$$

The eigen linear forms evaluated to $\Delta U = (\Delta\alpha_1, \Delta Y_1, \Delta\tau, \Delta u, \Delta e)^T$ are, setting

$$\Theta = -\frac{p_\varepsilon \Delta e - p_\varepsilon u \Delta u + p_{\alpha_1}\Delta\alpha_1 + p_\tau \Delta\tau + p_Y \Delta Y}{C^2}$$
$$\Phi = \frac{\Delta u}{C},$$

$$X = \sum_1^5 \ell_i(X) R_i$$

with

$$\ell_1 = \tfrac{1}{2}(\Theta + \Phi), \qquad \ell_2 = \tfrac{1}{2}(\Theta - \Phi)$$

$$\ell_3 = \frac{\frac{K}{\tau}\Theta - \Delta\alpha_1}{p_\varepsilon}, \quad \ell_4 = -\frac{\Delta Y_1}{p_\varepsilon}, \qquad \ell_5 = -\frac{\frac{\Delta p}{C^2} + \Delta\tau}{p_\varepsilon}$$

3.3 Several relations on the Lagrangian sound speeds

In this section, we provide several equivalent formulas on the Lagrangian speed of sound. They are the key to design the Roe average. We first give the values of the partial derivatives of the pressure with respect to Y_1, α_1, τ and ϵ in function of the partial derivatives of p_i, $i = 1,2$. Since $p_i = p_i(\varepsilon_i, \tau_i)$, we write

$$dp_i = \kappa_i d\varepsilon_i + \chi_i d\tau_i,$$

so that $d\varepsilon_i = \frac{1}{\kappa_i} dp_i - \frac{\chi_i}{\kappa_i} d\tau_i$. Since $\varepsilon = Y_1 \varepsilon_1 + Y_2 \varepsilon_2$, we have

$$\begin{aligned} d\varepsilon &= Y_1 d\varepsilon_1 + Y_2 d\varepsilon_2 + (\varepsilon_1 - \varepsilon_2) dY_1 \\ &= \left(\frac{Y_1}{\kappa_1} + \frac{Y_2}{\kappa_2}\right) dp - Y_1 \frac{\chi_1}{\kappa_1} d\tau_1 - Y_2 \frac{\chi_2}{\kappa_2} d\tau_2 + (\varepsilon_1 - \varepsilon_2) dY_1 \end{aligned}$$

Then we have $Y_i\tau_i = \alpha_i\tau$[†] so that

$$d\tau_i = -\frac{\tau_i}{Y_i}dY_i + \frac{\alpha_i}{Y_i}d\tau + \frac{\tau}{Y_i}d\alpha_i.$$

We replace $d\tau_i$ by this relation in the expression of $d\varepsilon$, so that

$$\begin{aligned} d\varepsilon = &\left(\frac{Y_1}{\kappa_1}+\frac{Y_2}{\kappa_2}\right)dp + \left(\frac{\chi_1\tau_1}{\kappa_1}-\frac{\chi_2\tau_2}{\kappa_2}+\varepsilon_1-\varepsilon_2\right)dY_1 \\ &-\left(\frac{\alpha_1\chi_1}{\kappa_1}+\frac{\alpha_2\chi_2}{\kappa_2}\right)d\tau + \tau\left(\frac{\chi_1}{\kappa_1}-\frac{\chi_2}{\kappa_2}\right)d\alpha_1. \end{aligned}$$

Since $dp = p_\varepsilon d\varepsilon + p_\tau d\tau + p_Y dY_1 + p_{\alpha_1} d\alpha_1$, we have

$$\begin{aligned} \frac{1}{p_\varepsilon} &= \frac{Y_1}{\kappa_1}+\frac{Y_2}{\kappa_2} \\ p_\tau &= p_\varepsilon\left(\frac{\alpha_1\chi_1}{\kappa_1}+\frac{\alpha_2\chi_2}{\kappa_2}\right) \\ p_{\alpha_1} &= p_\varepsilon\tau\left(\frac{\chi_2}{\kappa_2}-\frac{\chi_1}{\kappa_1}\right) \\ p_Y &= p_\varepsilon\left(\frac{\chi_2\tau_2}{\kappa_2}-\frac{\chi_1\tau_1}{\kappa_1}+\varepsilon_2-\varepsilon_1\right). \end{aligned} \tag{3.3}$$

The first result is the following:

Lemma 3.1. Defining

$$K = \frac{\alpha_2\frac{C_2^2}{Y_2}-\alpha_1\frac{C_2^2}{Y_1}}{\frac{C_2^2}{Y_2}+\frac{C_2^2}{Y_1}} = \frac{\rho_2 a_2^2-\rho_1 a_1^2}{\frac{\alpha_1}{\rho_1 a_1^2}+\frac{\alpha_2}{\rho_2 a_2^2}},$$

we have

$$\begin{aligned} C_1^2(\alpha_1+K) &= Y_1 C^2 \\ C_2^2(\alpha_2-K) &= Y_2 C^2 \end{aligned}$$

This lemma is itself a consequence of the following algebraic relations:

Lemma 3.2. For any U_i, α_i, i=1,2, we have

$$\begin{aligned} U_1\left(\alpha_1+\frac{U_2-U_1}{\frac{U_1}{\alpha_1}+\frac{U_2}{\alpha_2}}\right)-\alpha_1\frac{1}{\frac{U_1}{\alpha_1}+\frac{U_2}{\alpha_2}} &= \frac{\alpha_1(\alpha_1+\alpha_2-1)}{\frac{U_1}{\alpha_1}+\frac{U_2}{\alpha_2}} \\ U_2\left(\alpha_2-\frac{U_2-U_2}{\frac{U_1}{\alpha_1}+\frac{U_2}{\alpha_2}}\right)-\alpha_2\frac{1}{\frac{U_1}{\alpha_1}+\frac{U_2}{\alpha_2}} &= \frac{\alpha_2(\alpha_1+\alpha_2-1)}{\frac{U_1}{\alpha_1}+\frac{U_2}{\alpha_2}} \end{aligned} \tag{3.4}$$

Proof of lemma 3.2. It is a simple calculation. □

Proof of lemma 3.1. Taking $U_1 = \frac{C_1^2}{\alpha_1}$, $U_2 = \frac{C_2^2}{\alpha_2}$, using $\alpha_1+\alpha_2 = 1$ in (3.4), we obtain the result. □

Lemma 3.3.

[†]Note this is a quadratic relation, this is important for the derivation of the Roe average.

Let us recall the Lagrangian speed of sound:

$$C_i^2 = pp_{\varepsilon_i} - p_{\tau_i}.$$

The next result show that

$$C^2 = pp_\varepsilon - p_\tau + \frac{K}{\tau} p_{\alpha_1}.$$

The proof is purely algebraic, and only use lemma 3.1.

If

$$\tilde{C}^2 = pp_\varepsilon - p_\tau + \frac{K}{\tau} p_{\alpha_1},$$

then

$$\tilde{C} = C.$$

Proof. We first evaluate $pp_\varepsilon - p_\tau$ using $\frac{\chi_i}{\kappa_i} = p - \frac{C_i^2}{\kappa_i}$:

$$\begin{aligned} p - \frac{p_\tau}{p_\varepsilon} &= p - \alpha_1 \frac{\chi_1}{\kappa_1} - \alpha_2 \frac{\chi_2}{\kappa_2} \\ &= p - \alpha_1 \left(p - \frac{C_1^2}{\kappa_1} \right) - \alpha_2 \left(p - \frac{C_2^2}{\kappa_2} \right) \\ &= \alpha_1 \frac{C_1^2}{\kappa_1} + \alpha_2 \frac{C_2^2}{\kappa_2}. \end{aligned}$$

Hence, using again the same relation on the Lagrangian speed of sounds:

$$\begin{aligned} \frac{\tilde{C}^2}{p_\varepsilon} &= \alpha_1 \frac{C_1^2}{\kappa_1} + \alpha_2 \frac{C_2^2}{\kappa_2} - \frac{\chi_1}{\kappa_1} K + \frac{\chi_2}{\kappa_2} K \\ &= \frac{C_1^2}{\kappa_1} (\alpha_1 + K) + \frac{C_2^2}{\kappa_2} (\alpha_2 - K) \end{aligned}$$

Using lemma 3.1, this simplifies into

$$\frac{\tilde{C}^2}{p_\varepsilon} = \frac{C^2}{p_\varepsilon}$$

which ends the proof. □

Note again that the proof does not depend on the form of the equation of state, once the partial derivatives of the phase pressure are defined, thanks to (3.4).

3.4 Linearisation

We are looking for a linearisation that provide the same shock relations. We are looking for $\overline{A}$

$$\overline{A} = \begin{pmatrix} 0 & 0 & 0 & -\overline{K}/\bar{\tau} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ \overline{p_{\alpha_1}} & \overline{p_{Y_1}} & \overline{p_\tau} & -\overline{p_\varepsilon}\,\overline{u} & \overline{p_\varepsilon} \\ \bar{u}\,\overline{p_\alpha} & \bar{u}\,\overline{p_{Y_1}} & \bar{u}\,\overline{p_\tau} & \bar{p} - \overline{p_\varepsilon}(\bar{u})^2 & \bar{u}\,\overline{p_\varepsilon} \end{pmatrix}. \tag{3.5}$$

so that all the algebra on the eigenvalue and the eigenvectors obtained in the continuous case can be transposed. If we are able to define coefficients such that

$$\Delta p = \overline{p_{\alpha_1}} \Delta \alpha_1 + \overline{p_{Y_1}} \Delta Y_1 + \overline{p_\tau} \Delta \tau + \overline{p_\varepsilon} \Delta \epsilon \tag{3.6}$$

hold true, then automatically, we get the right jump relations on the conservative equations:

$$\begin{aligned}
&\Delta u = \Delta u\\
&\Delta p = \overline{p_{\alpha_1}}\Delta\alpha_1 + \overline{p_{Y_1}}\Delta Y_1 + \overline{p_\tau}\Delta\tau - \overline{p_\varepsilon}\bar{u}\Delta u + \overline{p_\varepsilon}\Delta e\\
&\Delta(pu) = \bar{u}\overline{p_{\alpha_1}}\Delta\alpha_1 + \bar{u}\overline{p_{Y_1}}\Delta Y_1 + \bar{u}\overline{p_\tau}\Delta\tau\left(\bar{p} - \overline{p_\varepsilon}(\bar{u})^2\right)\Delta u + \bar{u}\overline{p_\varepsilon}\Delta e.
\end{aligned}$$

Here $\bar{u}$ is the arithmetic average. The first step is to find these coefficients. Following step by step the procedure in the continuous case, we assume to have averaged derivatives such that

$$\Delta p_i = \overline{p_{\varepsilon_i}}\Delta\epsilon_i + \overline{p_{\tau_i}}\Delta\tau_i.$$

Since $\varepsilon_i = Y_1\varepsilon_1 + Y_2\varepsilon_2$,

$$\begin{aligned}
\Delta\varepsilon &= \sum_i \left(\bar{Y}_i\Delta\varepsilon_i + \bar{\varepsilon}_i\Delta Y_i\right)\\
&= \frac{\Delta p}{\overline{p_\varepsilon}} - \sum_i \frac{\overline{p_{\tau_i}}}{\overline{p_{\varepsilon_i}}}\bar{Y}_i\Delta\tau_i + \sum \bar{\varepsilon}_i\Delta Y_i
\end{aligned}$$

where we have defined

$$\frac{1}{\overline{p_\varepsilon}} = \sum_i \frac{\bar{Y}_i}{\overline{p_{\varepsilon_i}}}$$

and $\bar{Y}_i$, $\bar{\varepsilon}_i$ are the arithmetic averages. Then we use again the quadratic relation $Y_i\tau_i = \alpha_i\tau$ to write

$$\bar{Y}_i\Delta\tau_i + \bar{\tau}_i\Delta Y_i = \bar{\alpha}_i\Delta\tau + \bar{\tau}\Delta\alpha_i$$

and then

$$\Delta\tau_i = \frac{\bar{\alpha}_i}{\bar{Y}_i}\Delta\tau + \frac{\bar{\tau}}{\bar{Y}_i}\Delta\alpha_i - \frac{\bar{\tau}_i}{\bar{Y}_i}\Delta Y_i$$

so that

$$\Delta\varepsilon = \frac{\Delta p}{\overline{p_\varepsilon}} - \left(\sum_i \frac{\overline{p_{\tau_i}}}{\overline{p_{\varepsilon_i}}}\bar{\alpha}_i\right)\Delta\tau - \sum_i \frac{\overline{p_{\tau_i}}}{\overline{p_{\varepsilon_i}}}\bar{\tau}\Delta\alpha_i + \sum_i\left(\bar{\varepsilon}_i + \frac{\overline{p_{\tau_i}}}{\overline{p_{\varepsilon_i}}}\bar{\tau}_i\right)\Delta Y_i.$$

We set

$$\frac{1}{\overline{p_\varepsilon}} = \sum_i \frac{\bar{Y}_i}{\overline{p_{\varepsilon_i}}} \tag{3.7a}$$

$$\overline{p_{Y_1}} = \overline{p_\varepsilon}\left(\bar{\varepsilon}_1 + \frac{\overline{p_{\tau_1}}}{\overline{p_{\varepsilon_1}}}\bar{\tau}_1 - \bar{\varepsilon}_2 + \frac{\overline{p_{\tau_2}}}{\overline{p_{\varepsilon_2}}}\bar{\tau}_2\right) \tag{3.7b}$$

$$\overline{p_\alpha} = \overline{p_\varepsilon}\left(\frac{\overline{p_{\tau_1}}}{\overline{p_{\varepsilon_1}}} - \frac{\overline{p_{\tau_2}}}{\overline{p_{\varepsilon_2}}}\right)\bar{\tau} \tag{3.7c}$$

$$\overline{p_\tau} = \overline{p_\varepsilon}\left(\sum_i \frac{\overline{p_{\tau_i}}}{\overline{p_{\varepsilon_i}}}\bar{\alpha}_i\right) \tag{3.7d}$$

Then we can use the results of the continuous case: if we define

$$\overline{K} = \frac{\bar{\alpha}_2\frac{\bar{C}_2^2}{\bar{Y}_2} - \bar{\alpha}_1\frac{\bar{C}_2^2}{\bar{Y}_1}}{\frac{\bar{C}_2^2}{\bar{Y}_2} + \frac{\bar{C}_2^2}{\bar{Y}_1}} \tag{3.8a}$$

with

$$\bar{C}_i^2 = \bar{p}\,\overline{p_{\varepsilon_i}} - \overline{p_{\tau_i}}. \tag{3.8b}$$

We see that the non zero eigenvalue of $\overline{A}$, i.e the average speed of sound $\bar{C}$, satisfies

$$\frac{1}{\bar{C}^2} = \frac{\bar{Y}_1}{\bar{C}_1^2} + \frac{\bar{Y}_2}{\bar{C}_2^2} = \bar{p}\,\overline{p_\varepsilon} - \overline{p_\tau} - \frac{\overline{K}}{\bar{\tau}}\overline{p_{\alpha_1}}. \tag{3.9}$$

A close look at the expression of $\overline{p_{\alpha_1}}$ shows that the value of $\bar{\tau}$ is somewhat arbitrary. What is important is that we use the same expression in (3.7c) and (3.9).

3.5 Study of the jump relations

Let us recall the left eigenvectors hit against a state $\Delta U = (\Delta\alpha_1, \Delta Y_1, \Delta\tau, \Delta u, \Delta\varepsilon)^T$:

$$\ell_1(\Delta U) = \frac{1}{2C}\left(\Delta u + \frac{\Delta p}{\bar{C}}\right), \qquad \ell_2(\Delta U) = \frac{1}{2C}\left(\Delta u - \frac{\Delta p}{\bar{C}}\right)$$

$$\ell_3(\Delta U) = -\frac{1}{\overline{p_\varepsilon}}\left(\frac{\bar{K}}{\bar{\tau}}\Delta p + \Delta\alpha_1\right), \quad \ell_4(\Delta U) = -\frac{1}{\overline{p_\varepsilon}}\Delta Y_1$$

$$\ell_5(\Delta U) = -\frac{1}{\overline{p_\varepsilon}}\left(\frac{\Delta p}{\bar{C}} + \Delta\tau\right)$$

We see that

$$(\Delta u)^2 - \Delta p \Delta\tau = \bar{C}^2 \ell_1(\Delta U)\ell_2(\Delta U) - \Delta p\, \ell_5(\Delta U). \tag{3.10a}$$

Then, using the linearisation of Δp_i (knowing $p_i = p$), we have

$$\begin{aligned}\Delta p &= \overline{p_{\varepsilon_i}}\Delta\epsilon_i + \overline{p_{\tau_i}}\Delta\tau_i \\ &= \overline{p_{\varepsilon_i}}(\Delta\epsilon_i + \bar{p}\Delta\tau_i) + (\overline{p_{\tau_i}} - \bar{p}\,\overline{p_{\varepsilon_i}})\Delta\tau_i\end{aligned}$$

Using the quadratic relation $\alpha_i\tau = Y_i\tau_i$, first with $i = 1$, we have first

$$\bar{Y}_1\Delta\tau_1 + \bar{\tau}_1\Delta Y_1 = \bar{\alpha}_1\Delta\tau + \bar{\tau}\Delta\alpha_1,$$

so that

$$\begin{aligned}\bar{Y}_1\Delta p &= \bar{Y}_1\overline{p_{\varepsilon_1}}(\Delta\epsilon_i + \bar{p}\Delta\tau_i) - \bar{C}_1^2(\bar{\alpha}_1\Delta\tau + \bar{\tau}\Delta\alpha_1 - \bar{\tau}_1\Delta y_1) \\ &= \bar{Y}_1\overline{p_{\varepsilon_1}}(\Delta\epsilon_i + \bar{p}\Delta\tau_i) - C_i^2\tau_i\Delta Y_1 - \bar{C}_i^2\bar{\alpha}_i(\Delta\tau + \frac{\Delta p}{\bar{C}^2}) + \frac{\bar{C}_i^2}{\bar{C}^2}\bar{\alpha}_1\Delta p \\ &\qquad - \bar{C}_i^2\bar{\tau}(\Delta\alpha_i + \frac{\bar{K}}{\bar{\tau}}\frac{\Delta p}{\bar{C}^2}) + \frac{\bar{C}_i^2}{\bar{C}^2}\Delta p \\ &= \bar{Y}_1\overline{p_{\varepsilon_1}}(\Delta\epsilon_i + \bar{p}\Delta\tau_i) - C_i^2\tau_i\Delta Y_1 - \bar{C}_i^2\bar{\alpha}_i(\Delta\tau + \frac{\Delta p}{\bar{C}^2}) - \bar{C}_i^2\bar{\tau}(\Delta\alpha_i + \frac{\bar{K}}{\bar{\tau}}\frac{\Delta p}{\bar{C}^2}) \\ &\qquad + \frac{\bar{C}_i^2}{\bar{C}^2}(\bar{\alpha}_1 + \bar{K})\Delta p\end{aligned}$$

Using again Lemma 3.1, we have

$$\frac{\bar{C}_i^2}{\bar{C}^2}(\bar{\alpha}_1 + \bar{K})\Delta p = \Delta p.$$

hence

$$0 = \bar{Y}_1\overline{p_{\varepsilon_1}}(\Delta\epsilon_i + \bar{p}\Delta\tau_i) - C_i^2\tau_i\Delta Y_1 - \bar{C}_i^2\bar{\alpha}_i(\Delta\tau + \frac{\Delta p}{\bar{C}^2}) - \bar{C}_i^2\bar{\tau}(\Delta\alpha_i + \frac{\bar{K}}{\bar{\tau}}\frac{\Delta p}{\bar{C}^2}) \tag{3.10b}$$

Similarly, starting from

$$\Delta p = \bar{\kappa}\Delta\varepsilon + \bar{\chi}\Delta\tau + \bar{p}_\alpha \Delta\alpha + \bar{p}_Y \Delta Y$$

and using the same type of algebra, we get

$$\Delta p + \bar{C}^2\Delta\tau = \bar{\kappa}\big(\Delta\varepsilon + \bar{p}\Delta\tau\big) + \bar{p}_\alpha\big(\Delta\alpha + \frac{\bar{K}}{\bar{\tau}}\frac{\Delta p}{\bar{C}^2}\big) + \bar{p}_Y\Delta Y_1 - \bar{p}_\alpha\frac{\bar{K}}{\bar{\tau}}\left(\frac{\Delta p}{\bar{C}^2} + \Delta\tau\right). \tag{3.10c}$$

The relations (3.10) shows that the Hugoniot relations are linear combinations of the ℓ_j, j=1, ..., 5.

3.6 Example of the stiffened gas

The equation of state is

$$\varepsilon_i = \frac{p + \gamma_i p_\infty^i}{\gamma_i - 1}\tau_i$$

and then

$$(\gamma_i - 1)\Delta\varepsilon_i = \overline{p + \gamma_i p_\infty^i}\Delta\tau + \bar{\tau}\Delta p,$$

so that

$$\overline{p_{\tau_i}} = \frac{\gamma_i - 1}{\bar{\tau}_i}, \quad \overline{p_{\varepsilon_i}} = \frac{\overline{p + \gamma_i p_\infty^i}}{\bar{\tau}}.$$

3.7 Summary

We define $\bar{Y}_i = \frac{(Y_i)_L + (Y_i)_R}{2}$, $\bar{p} = \frac{p_L + p_R}{2}$ and $\bar{\alpha}_i = \frac{(\alpha_i)_L + (\alpha_i)_R}{2}$. Then we get

$$\bar{C}_i^2 = \bar{p}\bar{\kappa}_i - \bar{\chi}_i$$

and define

$$\frac{1}{\overline{p_\varepsilon}} = \sum_i \frac{\bar{Y}_i}{\overline{p_{\varepsilon_i}}}, \qquad \overline{p_{Y_1}} = \overline{p_\varepsilon}\left(\bar{\varepsilon}_1 + \frac{\overline{p_{\tau_1}}}{\overline{p_{\varepsilon_1}}}\bar{\tau}_1 - \bar{\varepsilon}_2 + \frac{\overline{p_{\tau_2}}}{\overline{p_{\varepsilon_2}}}\bar{\tau}_2\right)$$

$$\overline{p_{\alpha_1}} = \overline{p_\varepsilon}\left(\frac{\overline{p_{\tau_1}}}{\overline{p_{\varepsilon_1}}} - \frac{\overline{p_{\tau_2}}}{\overline{p_{\varepsilon_2}}}\right)\bar{\tau}, \quad \overline{p_\tau} = \overline{p_\varepsilon}\left(\sum_i \frac{\overline{p_{\tau_i}}}{\overline{p_{\varepsilon_i}}}\bar{\alpha}_i\right)$$

The average speed of sound is defined by

$$\frac{1}{\bar{C}^2} = \frac{\bar{Y}_1}{\bar{C}_1^2} + \frac{\bar{Y}_2}{\bar{C}_2^2} = \bar{p}\,\overline{p_\varepsilon} - \overline{p_\tau} - \frac{\overline{K}}{\bar{\tau}}\overline{p_\alpha},$$

and then

$$\overline{K} = \frac{\bar{\alpha}_2\frac{\bar{C}_2^2}{\bar{Y}_2} - \bar{\alpha}_1\frac{\bar{C}_2^2}{\bar{Y}_1}}{\frac{\bar{C}_2^2}{\bar{Y}_2} + \frac{\bar{C}_2^2}{\bar{Y}_1}}$$

The eigenvectors are

- eigenvalue C,

$$R_1 = \begin{pmatrix} -\bar{K}/\bar{\tau} \\ 0 \\ -1 \\ \bar{C} \\ \bar{p} + \bar{u}\,\bar{C} \end{pmatrix}$$

- eigenvalue $-C$,

$$R_2 = \begin{pmatrix} -\bar{K}/\bar{\tau} \\ 0 \\ -1 \\ -\bar{C} \\ \bar{p} - \bar{u}\,\bar{C} \end{pmatrix}$$

- eigenvalues $\lambda = 0$,

$$R_3 = \begin{pmatrix} -\overline{p_\varepsilon} \\ 0 \\ 0 \\ 0 \\ \overline{p_{\alpha_1}} \end{pmatrix}, \qquad R_4 = \begin{pmatrix} 0 \\ -\overline{p_\varepsilon} \\ 0 \\ 0 \\ \overline{p_Y} \end{pmatrix}, \qquad R_5 = \begin{pmatrix} 0 \\ 0 \\ -\overline{p_\varepsilon} \\ 0 \\ \overline{p_\tau} \end{pmatrix}$$

The linear forms applied to $\Delta U = (\Delta\alpha_1, \Delta Y_1, \Delta\tau, \Delta u, \Delta e)^T$ are

$$\ell_1 = \tfrac{1}{2}\left(\frac{\Delta p}{\bar{C}^2} + \frac{\Delta u}{\bar{C}}\right), \qquad \ell_2 = \tfrac{1}{2}\left(\frac{\Delta p}{\bar{C}^2} - \frac{\Delta u}{\bar{C}}\right)$$

$$\ell_3 = -\frac{1}{\overline{p_\varepsilon}}\left(\frac{\bar{K}}{\bar{\tau}}\frac{\Delta p}{\bar{C}^2} + \Delta\alpha_1\right), \quad \ell_4 = -\frac{\Delta Y}{\overline{p_\varepsilon}},$$

$$\ell_5 = -\frac{1}{\overline{p_\varepsilon}}\left(\frac{\Delta p}{\bar{C}^2} + \Delta\tau\right)$$

3.8 From Lagrangian to Eulerian coordinates

We proceed as in [**?**, **?**]. In order to explain the method, we begin with the continuous case, then we switch to the discrete one. In Euler coordinates, the system writes

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0, \qquad \frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} - K\frac{\partial u}{\partial x} = 0$$

with $U = (\rho Y_1, \rho, \rho u, E)^T$ and $F(U) = (\rho u Y_1, \rho u, \rho u^2 + p, u(E+p))^T$. Then we set $U = \rho n + U_0$ with $n = (0,1,0,0)^T$, $U_0 = \rho(Y_1, 0, u, e)^T$ and $F = uU + G_0$ with $G_0 = (0,0,p,pu)^T$.

In Lagrangian coordinate, the system writes

$$\frac{\partial W}{\partial t} + \frac{\partial G}{\partial m} = 0, \qquad \frac{\partial \alpha_1}{\partial t} = \frac{K}{\tau}\frac{\partial u}{\partial m}$$

with $W = \tau n + \tau U_0$ and $G = G_0 - un$. We follow step by step Gallice [**?**, **?**]:

$$dF = udU + Udu + dG_0 = udU + Udu + d_U G_0 + p_{\alpha_1} J d\alpha_1,$$

where $d_U G_0$ represents the differential with respect to the variable U and J is the 5×5 matrix which only non zero terms are $J_{4,1} = 1$ and $J_{5,1} = u$. We also set $W_U = \dfrac{\partial W}{\partial U}$ and $U_W = (W_U)^{-1}$. Then

$$\begin{aligned} W_U\Big(udU + Udu + dG_0\Big) &= W_U\Big(udU + Udu + d_U G_0 + p_{\alpha_1} J d\alpha_1\Big) \\ &= udW + W_U\, Udu + W_U\, d_U G_0 + p_{\alpha_1} W_U\, J d\alpha_1 \\ &= \left(uId + \frac{A_L}{\rho}\right) dW + \frac{p_{\alpha_1}}{\rho} J d\alpha_1 \end{aligned} \tag{3.11}$$

because

$$\frac{\partial W}{\partial U}J=\frac{1}{\rho}J.$$

Knowing that W does not depend on α_1, we obtain

$$d_UW=-\frac{W}{\rho}d\rho+\frac{d_UU_0}{\rho},$$

and hence

$$W_UU=-\frac{n}{\rho},\qquad W_U\,d_UG_0=\frac{d_UG_0}{\rho}.$$

Then, we get

$$ud\alpha_1-\frac{K}{\rho}d(\rho u)+\frac{K}{\rho}ud\rho=ud\alpha_1-Kdu,$$

where (denoting by $\mathbf{0}_{p,q}$ the $p\times q$ zero matrix, $\mathbf{l}=(0,uK/\rho,-K/\rho,0)$ and by abuse of language $\mathbf{J}=(0,0,p_{\alpha_1},up_{\alpha_1})^T$)

$$A^E=\begin{pmatrix}u & \mathbf{l}\\ \mathbf{J} & u\,\mathrm{Id}+\frac{1}{\rho}W_UA_U^LU_W\end{pmatrix}=u\mathrm{Id}+\begin{pmatrix}1 & \mathbf{0}_{1,4}\\ \mathbf{0}_{4,1} & W_U\end{pmatrix}A_L\begin{pmatrix}1 & \mathbf{0}_{1,4}\\ \mathbf{0}_{4,1} & U_W\end{pmatrix}\tag{3.12}$$

as in the conservative case. In the relation (3.12), A_U^L is the 4×4 matrix that corresponds to the components of W.

In the discrete case, we proceed along the same lines. We introduce a blending parameter a, and define the two averages

$$f^a=af_L+(1-a)f_R,\qquad f_a=(1-a)f_L+af_R,$$

so that

$$\Delta(fg)=f^a\Delta g+g_a\Delta f.$$

We immediately get

$$\Delta\begin{pmatrix}\alpha\\ \rho Y\\ \rho\\ \rho u\\ E\end{pmatrix}=\begin{pmatrix}1 & 0 & 0 & 0 & 0\\ 0 & \rho_a & -\frac{Y^a}{\underline{\rho^2}} & 0 & 0\\ 0 & 0 & -\frac{u^a}{\underline{\rho^2}} & \rho_a & 0\\ 0 & 0 & -\frac{e^a}{\underline{\rho^2}} & 0 & \rho_a\end{pmatrix}\Delta\begin{pmatrix}\alpha\\ Y\\ \tau\\ u\\ e\end{pmatrix}.$$

Then, we define

$$\overline{U_W}:=\begin{pmatrix}1 & 0 & 0 & 0 & 0\\ 0 & \rho_a & -\frac{Y^a}{\underline{\rho^2}} & 0 & 0\\ 0 & 0 & -\frac{u^a}{\underline{\rho^2}} & \rho_a & 0\\ 0 & 0 & -\frac{e^a}{\underline{\rho^2}} & 0 & \rho_a\end{pmatrix},\qquad \overline{W_U}:=\left(\overline{U_W}\right)^{-1}.$$

In order to simplify the algebra, we set

$$a=\frac{\sqrt{\rho_L}}{\sqrt{\rho_R}+\sqrt{\rho_L}}$$

and thus

$$\Delta F = \Delta\big(uU + G_0\big) = \overline{u}\Delta U + \underline{U}\Delta u + \Delta G_0$$
$$= \overline{u}\Delta U + \underline{U}\Delta u + \Delta_U G_0 + \overline{p_{\alpha_1}}\overline{J}\Delta\alpha_1$$

Here, $\overline{p_{\alpha_1}}$ and $\overline{J}$ are obtained via the Lagrangian averages. Some more algebra provides

$$\overline{U_W}\big(\overline{u}\Delta U + \underline{U}\Delta u + \Delta_U G_0 + \overline{p_{\alpha_1}}\overline{J}\Delta\alpha_1\big)$$
$$= \big(\overline{u}Id + \frac{1}{\underline{\rho}}\overline{A}_L\overline{W_U}\big)\Delta W + \frac{1}{\rho_a}\overline{J}\Delta\alpha_1$$

because: first, for any u, ρ, Y, v,

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \rho & -\frac{Y}{\rho^2} & 0 & 0 \\ 0 & 0 & -\rho^{-2} & 0 & 0 \\ 0 & 0 & -\frac{u}{\rho^2} & \rho & 0 \\ 0 & 0 & -\frac{e}{\rho^2} & 0 & \rho \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ v & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \rho^{-1} & 0 & 0 & 0 & 0 \\ \frac{v}{\rho} & 0 & 0 & 0 & 0 \end{pmatrix}$$

and second,

$$\overline{W_U}\underline{U} = -\frac{n}{\underline{\rho}}, \qquad \overline{W_U}\Delta_U G_0 = \frac{\Delta_U G_0}{\underline{\rho}}.$$

These relations originates from

$$\Delta\rho W = \Delta(n + U_0) = \underline{\rho}\Delta W + \overline{W}\Delta\rho$$

and then

$$\Delta W = -\frac{\overline{W}}{\underline{\rho}}\Delta\rho + \frac{\Delta U_0}{\underline{\rho}}$$

Similarly, since $\Delta(\rho u) = \underline{\rho}\Delta u + \overline{u}\Delta\rho$, we have

$$\Delta u = \frac{1}{\underline{\rho}}\Delta(\rho u) - \frac{\overline{u}}{\underline{\rho}}\Delta\rho,$$

and then

$$\frac{\overline{K}}{\tau}\Delta u = \frac{\overline{K}}{\tau}\frac{1}{\underline{\rho}}\Delta(\rho u) - \frac{\overline{K}}{\tau}\frac{\overline{u}}{\underline{\rho}}\Delta\rho,$$

We finally obtain an average for the Eulerian system by taking

$$\overline{A_E} = \overline{u}\,\mathbf{Id} + \frac{1}{\underline{\rho}}\overline{U_W A_L}\,\overline{W_U}.$$

The two matrices are simultaneously diagonalisable in $\mathbb{R}$ with real eigenvalues.

3.9 Numerical approximation

3.9.1 Roe scheme

In the conservative case, and first order in space, the Roe scheme has two equivalent formulations,

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left(F^{Roe}(U_{i+1}^n, U_i^n) - F^{Roe}(U_i^n, U_{i-1}^n)\right)$$

with

$$F^{Roe}(U,V)=\frac{1}{2}\Big(F(U)+F(V)-|\bar{A}(U,V)|(V-U)\Big)$$

or the fluctuation form:

$$U_i^{n+1}=U_i^n-\frac{\Delta t}{\Delta x}\Big(\Phi_-(U_i^n,U_{i+1}^n)+\Phi_+(U_{i-1}^n,U_i^n)\Big) \tag{3.13a}$$

with

$$\Phi_-(U,V)=\bar{A}(U,V)^-(V-U), \qquad \Phi_+(U,V)=\bar{A}(U,V)^+(V-U). \tag{3.13b}$$

We note that conservation holds true if (and only if)

$$\Phi_-(U,V)+\Phi_+(U,V)=\bar{A}(U,V)(V-U).$$

Roe scheme is known for not being entropy satisfying. This cured by standard entropy fix: we estimate the positive and negative part of the eigenvalues of the Roe matrix with Harten-Yee entropy fix:

$$x^+\approx\frac{x+\varphi(x)}{2}$$
$$x^-\approx\frac{x-\varphi(x)}{2}$$

with

$$\varphi(x)=\begin{cases} |x| & \text{if } |x|>\varepsilon \\ \frac{x^2+\varepsilon^2}{2\varepsilon} & \text{else}\end{cases}$$

We take $\varepsilon=0.05$.

In the non conservative case, we generalize the relation (3.13). This formalism is linked to the Roe's fluctuation splitting form (see [?, ?]), also called residual distribution schemes [?]. They also have the same form as the path conservative schemes (see [?]), but here we do no consider any path Γ to evaluate

$$\int_\Gamma A(U)\frac{\partial U}{\partial x}dx$$

which is equal to $\Phi_-(U,V)+\Phi_+(U,V)$ for path conservative schemes.

The second order extension is done following Roe's idea (see [?]), section 4.2, with superbee limiter. This is not essential for our discussion, but this example is interesting for showing the robustness of the limitation procedure.

3.9.2 A hybrid scheme

As is shown in the numerical results, the Roe scheme derived in the previous section cannot efficiently solve any non conservative Riemann problem. This is not a particular drawback of the Roe scheme, or that particular version, but a general drawback of any finite difference type method.

The explanation of this known phenomena is rather simple. Assume a finite difference scheme that we put in a residual distribution form,

$$U_i^{n+1}=U_i^n-\frac{\Delta t}{\Delta x}\Big(\Phi_i^{i+1/2}+\Phi_i^{i-1/2}\Big). \tag{3.14}$$

If the problem where in conservative form, with a numerical flux $F_{i+1/2}$, the residual would be

$$\Phi_i^{i+1/2}=F_{i+1/2}-F_i, \qquad \Phi_{i+1}^{i+1/2}=F_{i+1}-F_{i+1/2}.$$

For the Roe scheme, the residual write

$$\Phi_i^{i+1/2} = \overline{A}(U_i,U_{i+1})^-(U_{i+1}-U_i), \qquad \Phi_{i+1}^{i+1/2} = \overline{A}(U_i,U_{i+1})^+(U_{i+1}-U_i).$$

If one evaluates the equivalent equation of the scheme (3.14), one gets

$$\frac{\partial U}{\partial t} + A(U)\frac{\partial U}{\partial x} = \mathcal{D}\left(U, \frac{\partial U}{\partial x}\right) + O(\Delta x^2)$$

where $\mathcal{D}\left(U, \frac{\partial U}{\partial x}\right)$ is a second order (elliptic) operator of the form, in the present case,

$$\mathcal{D}(U, \frac{\partial U}{\partial x}) = \begin{pmatrix} \Delta x \theta \frac{\partial}{\partial x}\left(d\frac{\partial \alpha_1}{\partial x}\right) \\ \Delta x \frac{\partial}{\partial x}\left(D\frac{\partial V}{\partial x}\right) \end{pmatrix}, \qquad \text{with } V = (\tau, u, e)^T$$

where D is a 3×3 matrix, d and θ non zero scalars. The precise form of D, d, θ depends on the particular scheme. If we were able to compute the traveling waves solution of the Riemann problems for the modified equation, the form of the solution depends on the parameters and matrices that defines the dissipative operator. Since $\theta \neq 0$, the end states also depends on them, the shape of the traveling wave is important, contrarily to what happens in the conservative case. In other words, the entropy created across a numerical shock wave depends strongly on the precise form of the numerical dissipation.

One way to avoid this is to design a scheme so that the true dissipation mechanism is imitated, but again there will be higher order terms in the expansions: if the shock waves are strong enough, then it is easy to find examples for which the numerical solution will not converge to the exact one. It is enough to find a strong enough shock. This approach has been taken in Karni [**?**,**?**] and more recently in Mishra et al [**?**,**?**] for single phase of multiphase flows.

Indeed the only way to solve the problem of finding a scheme which converge for sure to the exact solutions, at least for Riemann problem, is to avoid any numerical diffusion across shocks.

One way of doing so is to use the Glimm scheme. We use the standard procedure [**?**] after having noticed it only need the knowledge of the solution of the Riemann problem. Since here we know the jump relations and the Riemann invariant, this is doable. As recalled in the numerical section, this leads to solutions with an excellent resolution of the shock and contact, but a bit noisy in the regular part of the solution.

In order to overcome this problem, we have also set up a hybrid scheme: for each time step, we first compute a shock indicator, here

$$\theta_i^n = \min\Big((p_i^n - p_{i+1}^n)(u_i^n - u_{i+1}^n), (p_i^{n+1} - p_{i+1}^{n+1})(u_i^{n+1} - u_{i+1}^{n+1})\Big)$$

If $\theta_i^n > 0$ then U_i^{n+1} is the Glimm solution, else we take the Roe solution.

4 Numerical results

We evaluate the three schemes (Roe, Glimm and hybrid scheme) on three problems. In each case, the Roe scheme is second order with superbee limiter. The CFL is set to 0.4 because of Glimm' scheme.

The first two problems are Riemann problems. In the first one, the initial velocities are null, and for the second one, the initial velocities have opposite sign and large absolute values. In both cases, all the variables are initially discontinuous, including the mass fraction. The last case is a shocked nozzle flow problem: the solution is nowhere constant, in particular before and after the shock wave. In the three cases, the fluids are governed by the stiffened EOS with the parameters given in table 1. We have chosen very strong shock tube problems instead of

	Fluid 1	fluid 2
p_∞ (Pa)	0	6.10^8
γ	1.4	4.4

Table 1: Parameters for the stiffened EOS.

less strong ones in order to show the robustness of our approach.

4.1 Test case # 1

The initial conditions are given in table 2. The jump in pressure is very large across the shock. Similar cases have been considered in [?, ?, ?].

	α	ρ_1 (kg/m^3)	ρ_2 (kg/m^3)	u (m/s)	p (Pa)
Left	0.2954	1185	3622	0	2.10^{11}
Right	0.7954	1185	3622	0	1.10^5

Table 2: Initial condition for test case # 1.

The different solutions are given in Figure 1. The zoom of the solutions near the fan (to see better the differences) are given in Figure 2. The Roe scheme reproduces the fan very well (remember this is a second order scheme with superbee limiter), but is completely off across the shock wave as expected. The Glimm scheme is very good for the shock wave but provides a noisy solution, as expected, in the fan. The hybrid scheme takes the best qualities of the Roe scheme and the Glimm scheme: the fan is very good, as well as the shock structure. Here the mesh is uniform with 100 cells on a tube of 1 m long.

On Figure 1 and 2, one may observe a shift between the different curves. The exact solution is plotted with 1000 points, and the numerical ones are obtained with 100 points only. The shift is only 1-2 Δx. For Glimm's scheme, it is known that the quality of the random generator plays an important role, see [?], hence this remark holds true for the hybrid scheme too. Here we have used the intrinsic Fortran 90 `MRANDOM`, with a seed that changes at every time step. Concerning the Roe scheme in the fan parts, we can see an effect of the numerical dissipation: the solution is a bit off by 1-2 grid points from the exact one. They match well in the middle of the fan, remember that only 100 grid points are used in the simulation. We have also checked that when we increase the number of grid points, the shift still exists, but it remains 1-2 mesh points. We have run up to 10^4 grid points, the results are not reported. hence, we are quite confident with these results. The same remark applies to each of the test cases reported in this paper.

4.2 Test case # 2

In this case, the thermodynamic quantities are the same as in test case #1, as well as the mesh, but the velocity are of opposite sign and of quite large velocity, see table 3. These conditions

	α	ρ_1 (kg/m^3)	ρ_2 (kg/m^3)	u (m/s)	p (Pa)
Left	0.2954	1185	3622	1000	2.10^{11}
Right	0.7954	1185	3622	-2000	1.10^5

Table 3: Initial condition for test case # 2.

leads to a very strong shock wave (differential in velocity ≈ 2500 m/s and $9\ 10^{11}$ Pa) and a small but stiff fan. The results are given on Figures 3 and some details on Figures 4.

Again, we see that the Roe solution is different from the exact one, but here the difference is barely visible. For example, the exact volume fraction (usually the most sensitive quantity) across the contact discontinuity is

$$\alpha_{ex}^{L,\star} = 0.29594268, \qquad \alpha_{ex}^{R,\star} = 0.78670510$$

while the numerical ones are

$$\alpha_{Roe}^{L,\star} = 0.295945, \qquad \alpha_{Roe}^{R,\star} = 0.7863.$$

The velocities are:

$$u_{ex}^{L} = 0.13026712\,10^4, \qquad u_{Roe}^{\star} = 0.13039\,10^4.$$

4.3 Nozzle flow problem

Assuming a two dimensional flow in a smooth nozzle (along the x axis), and a solution that depends weakly on the y component, we the flow variable satisfy the following system

$$\begin{aligned}
\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} &= K\frac{\partial u}{\partial x} + \frac{u\alpha_1}{A}\frac{\partial A}{\partial x} = 0\\
\frac{\partial \rho_1\alpha_1}{\partial t} + \frac{\partial \rho_1\alpha_1 u}{\partial x} &= -\frac{\rho_1\alpha_1 u}{A}\frac{\partial A}{\partial x}\\
\frac{\partial \rho_2\alpha_2}{\partial t} + \frac{\partial \rho_2\alpha_2 u}{\partial x} &= -\frac{\rho_2\alpha_2 u}{A}\frac{\partial A}{\partial x}\\
\frac{\partial \rho u}{\partial t} + \frac{\partial(\rho u^2+p)}{\partial x} &= -\frac{\rho u^2}{A}\frac{\partial A}{\partial x}\\
\frac{\partial E}{\partial t} + \frac{\partial\big(u(E+p)\big)}{\partial x} &= -\frac{u(E+p)}{A}\frac{\partial A}{\partial x}
\end{aligned} \tag{4.1}$$

where A is the area.

The boundary conditions are

- the reservoir conditions are the volume fraction α_1, the mass fraction Y_1, the mass flow and the total enthalpy,
- the outflow conditions are given by the pressure p^{exit} because we have a subsonic outflow.

The values are given in Table 4. The derivation of (4.1) is recalled in appendix A.

We describe our numerical strategy. Let $U = (\alpha_1, \alpha_1\rho_1, \alpha_2\rho_2, \rho u, E)^T$ be the state variables. We consider a regular mesh $x_0 = x_{min}, \dots, x_j = x_0 + j\Delta x, \dots x_N = x_{max}$. The vector $U^n = (U_0^n, \dots U_N^n)$ represents the vector of state variables on the mesh at $t_n = n\Delta t$. We start from a scheme (Roe's, Glimm's, hybrid) which operator is $\mathcal{L}$, i.e.

$$U^{n+1} = \mathcal{L}(U^n).$$

	α_1	ρ_1 (Kg/m^3)	ρ_2 (Kg/m^3)	p (Pa)
Reservoir	0.95	1.0	1000	10^8
Exit	-	-	-	10^7

Table 4: Reservoir and conditions at the exit, subsonic case.

We have used a splitting strategy,

$$U^{n+1/2} = \mathcal{L}(U^n), \qquad U^{n+1} = U^{n+1/2} + \Delta t S^{n+1/2}$$

with $S^{n+1/2} = (S_0^{n+1/2}, \dots, S_N^{n+1/2})$ with

$$S_j^{n+1/2} = \begin{pmatrix} K_i^{n+1/2} u_i^{n+1/2} \\ -(\rho_1 \alpha_1 u)_j^{n+1/2} \\ -(\rho_2 \alpha_2 u)_j^{n+1/2} \\ -(\rho u^2)_j^{n+1/2} \\ -\Big(u(E+p)\Big)_i^{n+1/2} \end{pmatrix} \frac{1}{A_j}\frac{dA}{dx}(x_j).$$

The time accuracy has no importance since we are looking for a steady solution. The boundary conditions are strongly imposed (since we know the exact solution).

It is known that Glimm' scheme, with such a splitting strategy, has a poor behavior. This is known since [**?**], and an improved discretisation, using the solution of a Riemann problem with source does improve the solution, see [**?**]. Such a strategy could be implemented , with a priory an improved quality of solution. However, in the present case, the solution of this Riemann problem, though possible in principle, is quite cumbersome to get. In order to overcome this problem, we have used a large discretisation (1000 points).

In the case of the hybrid scheme, we need to detect the shock. Our criteria is $p_{i+1} - p_{i-1} \geq p_i/10$ and $u_{i+1} - u_{i-1} \leq u_i/10$. The geometry of the nozzle is, with $A_0 = 0.06406$:

- If $x \leq 1/2$, $a(x)/A_0 = 1 + 3(1/2 - x)^2$
- If $x \geq 1/2$, $a(x)/A_0 = 1 + 10(x - 1/2)^3 + 10(x - 1/2)^2$

The solutions are quite comparable to the exact solution. The most sensitive variable is the volume fraction. We see that the Roe scheme does not provide the correct solution: the level of the volume fraction, after the shock, is not correct. For the Glimm' scheme, we get the right levels, the location of the shock is within one mesh cell. The hybrid scheme provide similar answer. Note that the Roe scheme is obtained with the second order scheme.

5 Conclusion

We have derived a Roe average for compressible multiphase flow. This system is non conservative. Hence, our guiding principle is that the Roe matrix, which is of course diagonalisable in $\mathbb{R}$, admits a spectral decomposition which left eigenvectors provide the Hugoniot relations without any approximation. Unfortunately, the system is non conservative, and we show that a Glimm scheme permits to compute the exact solution of Riemann problems. As it is the case for the Glimm' scheme, the solution is a bit noisy, and we show that an hybridization with the previous Roe method enable to recover nicely the correct weak entropy solutions of the problem. We also explore what happens for nozzle flows, a more complex situation where the states are not constant before and after the shocks..

We have explained the procedure for *one* particular non conservative system equipped with jump relations. We believe that our procedure can be generalized to other systems. We believe also that the front tracking method would be another candidate for such an hybridation.

In this paper, we have consider very severe test cases. For example, the Remann problems have huge pressure/velocity jumps. Using this kind of test, it is easier to show the drawbacks of finite difference methods, and to illustrate the merit of our technique. Of course, for weak to moderate, any consistent method will do the job, as already noticed by [?].

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A Nozzle equations

The nozzle equations express that $D=\rho A u$, $H=\frac{E+p}{\rho}$ and the specific entropies stay constant. Similarly, the mass fraction stay constant, and the mass flow is constant. Using this, we immediately get

$$\frac{\partial \rho_i\alpha_i}{\partial t}+\frac{\partial}{\partial x}(\rho_i\alpha_i u)+\frac{\rho_i\alpha_i u}{A}\frac{dA}{dx}, \tag{A.1a}$$

$$\frac{\partial \rho u}{\partial t}+\frac{\partial}{\partial x}(\rho u^2+p)+\frac{\rho u^2}{A}\frac{\partial A}{\partial x}=0 \tag{A.1b}$$

and

$$\frac{\partial E}{\partial t}+\frac{\partial}{\partial x}\Big(u(E+p)\Big)+\frac{u(E+p)}{A}\frac{\partial A}{\partial x}=0 \tag{A.1c}$$

The equation on the mass fraction is a bit more subtle to get. Using of of the remarks in [?] that shows that the equation on the volume fraction is a consequence of the equality of the pressures for an isotropic flow, we evaluate the Lagrangian derivative of $p_1(\rho_1,e_1)=p(\rho_2,e_2)=p$. This gives, using Lagrangian derivative, and the fact that p_i do not depend on the entropy in that case:

$$\begin{aligned}\frac{d}{dt}p_1(\rho_1,s_1)-\frac{d}{dt}p_2(\rho_2,s_2)&=\frac{\partial p_1}{\partial \rho_1}\frac{d\rho_1}{dt}-\frac{\partial p_2}{\partial \rho_2}\frac{d\rho_2}{dt}\\&=a_1^2\frac{d\rho_1}{dt}-a_2^2\frac{d\rho_2}{dt}.\end{aligned} \tag{A.1d}$$

Then, using the mass conservation equations, we obtain

$$\frac{d(\alpha_i\rho_i)}{dt}=-\rho_i\alpha_i\frac{\partial u}{\partial x}-\frac{\rho_i\alpha_i u}{A}\frac{dA}{dx}.$$

Using the chain rule and (A.1d), we have

$$\frac{\partial \alpha_1}{\partial t}+u\frac{\partial \alpha_1}{\partial x}=K\frac{\partial u}{\partial x}+\frac{u}{A}\frac{\partial A}{\partial x} \tag{A.1e}$$

The boundary conditions are classical:

- Subsonic inflow. If ρ^1, u^1, p^1 are the values of the density, velocity and pressure at the point x_1, α^1 the value of the mass fraction of fluid # 1, and Y^1 its mass fraction at the same location (with a slight abuse of notations here), we state

$$\begin{aligned}&Y_1 = Y^\infty\\&s_1 = s^\infty, s_2 = s_2^\infty\\&H_1 = H^\infty\end{aligned}$$

  and impose the value of the Riemann invariant associated to the eigenvalue $u - c$.

- Supersonic outflow: we impose the exit pressure.

Details on the computation of the exact solutions can be found in [**?**].

α_1 p

ρ u

Y_1

Figure 1: Solution for the data #1. 100 grid points are used

α_1 p

ρ u

Figure 2: Zoom of the solution for the data #1.

α_1 p

ρ u

Y_1

Figure 3: Solution for the data # 2 .

α_1 p

ρ u

Figure 4: Zoom of the solution for the data # 2.

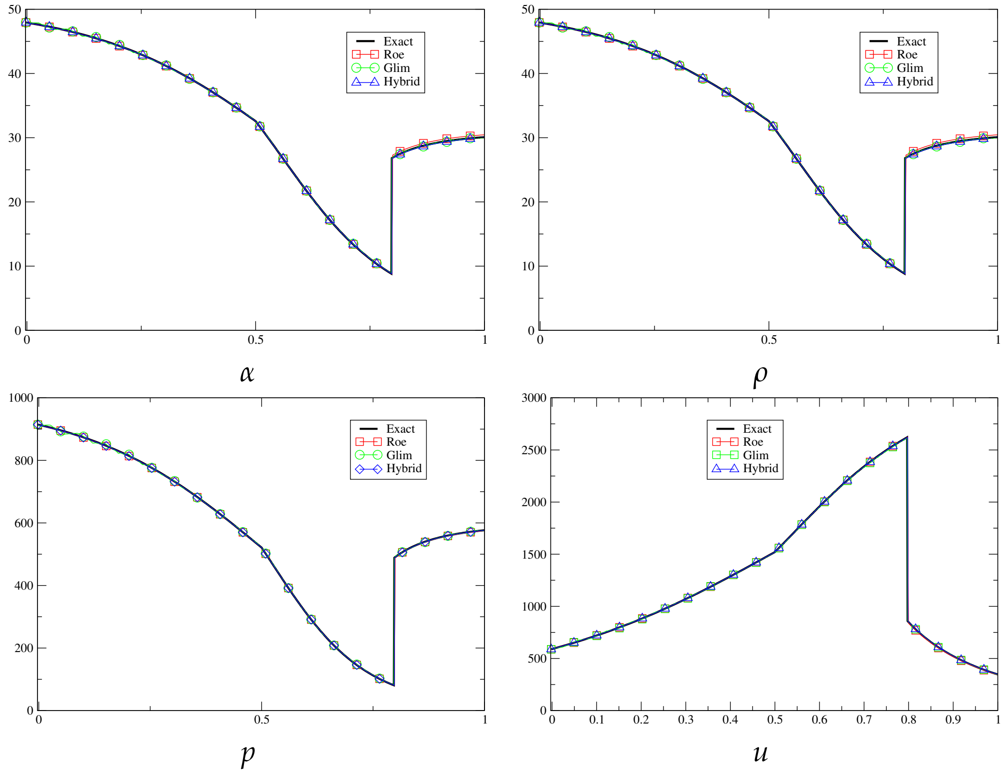

Figure 5: Global distribution of the physical variables: Exact, Roe scheme, Glimm and hybrid scheme.

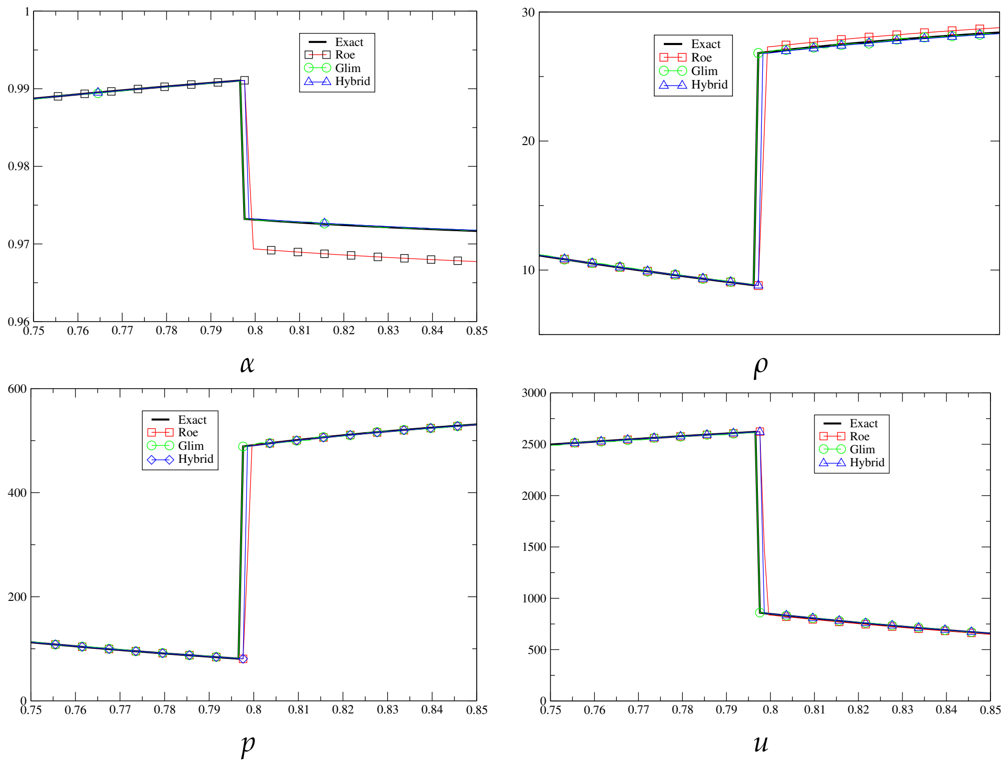

Figure 6: Zoom of the physical variable around the shock location.